Molecular dynamic study of diffusion systems confined to uni-directional zeolite structures

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A study of molecular dynamic simulation was conducted to investigate diffusion characteristics of guest molecules which diffuse into single-channel zeolites. Diffusion behaviours in a single channel pore, in general, exhibit three regimes which are (1) normal Fickian diffusion d ~ t (2) projectile diffusion d ~ t2 (3) single file diffusion d ~ t0.5 where d stands for mean square displacements of molecules (MSD).
We focused on studying diffusion behaviours with various types of zeolites and different lengths: different pore sizes and pore lengths.
We used one dimensional silicalite zeolites, TON and AFI, whose structures were obtained from the IZA databases. The pore size of AFI (7.3x7.3Å) is larger than that of TON (4.6x5.7Å). We performed molecular dynamics simulations with NVT ensemble.
It can be seen that variations in pore size and pore length have effect on diffusion characteristics of systems.